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A CLASSICAL MODEL OF FERROMAGNETISM AND ITS SUBSEQUENT QUANTIZI--ETC(U)

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A CLASSICAL MODEL OF FERROMAGNETISM AND ITS SUBSEQUENT QUANTIZING
IN THE AREA OF LOW TEMPERATURES

(Ein Klassisches Modell des Ferromagnetismus und seine nachtragliche
Quantisierung im Gebiete Tiefer Temperaturen)

by G./Heller H.A./Kramers

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Translated from: K. Akademie van Wetenschappen te Amsterdam.
Proceedings of the Section of Sciences 37,
pp 378-385, 1934, by

A complete translation from the German, by L. L. Lawrence.

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A CLASSICAL MODEL OF FERROMAGNETISM AND ITS SUBSEQUENT QUANTIZING
IN THE AREA OF LOW TEMPERATURES

Article by G. Heller and H. A. Kramers, Utrecht
-- Communicated at the Meeting of June 30, 1934.

AMSTERDAM ROYAL ACAD. SCI., Vol 37:378-385(1934).

1. Summary: The classical model of ferromagnetism is defined. Only in the case of the space lattice, it clearly results in ferromagnetic saturation. The simple quantizing of this model results exactly in the formulas of Bloch* and Møller**.

* Bloch, ZS. F. PHYSIK, Vol 61:206(1930) and Vol 74:295(1932).

** Møller, ZS. F. PHYSIK, Vol 82:559(1933).

2. Classical Theory of Ferromagnetism, Especially at Low Temperatures

We consider a lattice of N atoms. Let $\frac{\hbar}{2}\sigma_i$ be the operator of the mechanical moment, $\mu\sigma_i$ ($\mu = \frac{e\hbar}{mc2}$) the operator of the magnetic moment of the i-th atom. If \vec{H} is the external magnetic field strength, then the energy operator, as far as it is function of the spin moments:

$$W = -\mu\vec{H} \sum_{i=1}^N \vec{\sigma}_i - \frac{1}{2} \sum_{s,t} I_{st} (\vec{\sigma}_s \cdot \vec{\sigma}_t) \dots (1)$$

The I_{st} are exchange integrals between the atoms s and t.

If the eigenvalues E_z of this operator are known, the condition sum

$$Z(\theta, H) = \sum e^{-\frac{E_z}{kT}}; (\theta = kT) \dots (2)$$

can be calculated and the expected value of the magnetic moment

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$$\bar{\mu} = \theta \frac{\partial \ln Z}{\partial H} \dots \dots \dots (3)$$

is found.

With Heisenberg and Bloch, we assume that the I_{st} are different only for adjacent units of zero and we establish the same task as Bloch, -- the calculation of $\bar{\mu}$ for the linear chain, the square layer lattice and the cubic space lattice.

The "classical" treatment of the calculation consists of the fact that we consider the operators of equation (1) as c-numbers in the sense of classical mechanics. The vector s_i ($|s|=n$) with the directional cosines X_i, Y_i, Z_i ($X^2 + Y^2 + Z^2 = 1$) corresponds to the spin operator σ_i , and equation (1) is for the linear chain:

$$W = -\mu n H \sum_{k=1}^N Z_k - \frac{1}{2} I n^2 \sum_{k=1}^N (X_k X_{k+1} + Y_k Y_{k+1} + Z_k Z_{k+1}) \quad (4)$$

if we select the field direction as Z direction, whereby we set $X_{N+1} = X_1$ and so forth for the completion of the lattice.

We now obtain the condition sum through the integration of $e^{-\frac{W}{\theta}}$ through the canonical coordinates of the entire system. If, for example, we describe the spin orientation of the i-th atom by the canonical coordinates $\frac{\hbar}{2} s_{zi}$ and φ_i and introduce the differential of the space angle by

$$n d\omega_i = ds_{zi} d\varphi_i$$

we obtain the condition sum:

$$Z(\theta, H) = \left(\frac{\hbar}{2} n \right)^N \int e^{-\frac{W}{\theta}} d\omega_1 d\omega_2 \dots d\omega_N \dots \quad (5)$$

The exact evaluation of (5) presents considerable mathematical difficulties. We limit ourselves to the investigation of the behavior at low temperatures $\theta \ll I$.

We can then assume that almost all spins lie almost in the Z direction. We can then develop the energy W by powers of X_i and Y_i and we obtain with

$$\frac{\mu H}{nI} = a:$$

$$W = -Nn\left(\frac{nI}{2} + \mu H\right) + \frac{In^2}{2} \left[\sum_{i=1}^N (1+a)(X_i^2 + Y_i^2) - X_i X_{i+1} - Y_i Y_{i+1} \right] \quad (6)$$

$$d\omega_i = dX_i dY_i$$

$$Z = \left(\frac{\hbar}{2}n\right)^N \int_{-\infty}^{\infty} e^{-\frac{W}{\hbar}} dX_1 \dots dX_N dY_1 \dots dY_N.$$

In practice, the integrand is markedly different from 0 only when all X_i , Y_i have very small amounts. We may therefore extend the integration limits from $-\infty$ to $+\infty$ (This conclusion is of course only permissible when the integral remains convergent).

We apply the integral formula:

$$\int_{-\infty}^{\infty} e^{-\sum_{i,k} \sigma_{ik} X_i X_k} dX_1 dX_2 \dots dX_N = \pi^{\frac{N}{2}} |A|^{-\frac{1}{2}} = \prod_{\lambda=1}^N \sqrt{\frac{\pi}{\Delta_\lambda}}. \quad (7)$$

In it, σ_{ik} are the coefficients of a symmetrical matrix, $|A|$ is its determinant, Δ_λ ($\lambda=1\dots N$) are its eigenvalues.

Proof: There are real unitary matrices U, which transform A on principal axes:

$$U^{-1} A U = \Delta.$$

If we introduce new coordinates through:

$$X_i = \sum U_{ik} X'_k$$

we obtain:

$$\int_{-\infty}^{\infty} e^{-\sum \Delta_\lambda X_\lambda'^2} dX_1 \dots dX_N = \prod_{\lambda=1}^N \int_{-\infty}^{\infty} e^{-\Delta_\lambda X_\lambda'^2} dX_\lambda' = \prod_{\lambda=1}^N \sqrt{\frac{\pi}{\Delta_\lambda}}.$$

With (7), the condition sum becomes:

$$Z = e^{\frac{Nn}{\theta} \left(\frac{nI}{2} + \mu H \right)} \left(\frac{\bar{h}\theta}{In} \right)^N \frac{\pi^N}{\prod_i \Lambda_i} \dots \dots \dots (8)$$

The Λ_i are the eigenvalues of the square form within brackets in (6). They are found from the secular equations:

$$-\frac{1}{2} u_{i-1,i} + (1 + a - \Lambda_i) u_{i,i} - \frac{1}{2} u_{i+1,i} = 0 \dots \dots (9)$$

One solution is:

$$u_{i,i} = e^{\frac{2\pi i}{N} \lambda}, \Lambda_i = 1 + a - \cos \frac{2\pi}{N} \lambda \dots \dots \dots (10)$$

Equation (10) provides us with N independent eigenvectors, thus a complete system. We thus also know all eigenvalues and thus, according to (8), the condition sum:

$$\ln Z = \frac{Nn}{\theta} \left(\frac{nI}{2} + \mu H \right) + N \ln \frac{\bar{h}\pi\theta}{In} - \sum_{i=1}^N \ln \left(1 + a - \cos \frac{2\pi}{N} \lambda \right).$$

In the case of large numbers of atoms N, we can replace the sum by an integral through $\xi = \frac{2\pi}{N} \lambda$:

$$\ln Z = \frac{Nn}{\theta} \left(\frac{nI}{2} + \mu H \right) + N \ln \frac{\bar{h}\pi\theta}{In} - \frac{N}{2\pi} \int_0^{2\pi} \ln(1 + a - \cos \xi) d\xi. (11)$$

According to (3) and (11), the expected value of the magnetic moment becomes:

$$\begin{aligned} \bar{\mu} &= \theta \frac{\partial \ln Z}{\partial H} = Nn\mu - \frac{N}{2\pi} \frac{\mu\theta}{nI} \int_0^{2\pi} \frac{d\xi}{1 + a - \cos \xi} \\ &= Nn\mu - N \frac{\mu\theta}{nI} \frac{1}{\sqrt{a(a+2)}} \end{aligned}$$

This expression diverges with respect to $-\infty$ for $H \rightarrow 0$, i.e. $a \rightarrow 0$. This result does of course not have any physical significance, but it perhaps makes possible the conclusion that there is no tendency to ferromagnetism.

Analogous calculations apply to square layer and space lattices. The energy of the simple square layer lattice is:

$$W = -n\mu H \sum_{k,l=1}^N Z_{kl} - \frac{I}{2} n^2 \sum_{k,l=1}^N (X_{k,l} X_{k+1,l} + X_{k,l} X_{k,l+1} + Y_{k,l} Y_{k+1,l} + Y_{k,l} Y_{k,l+1} + Z_{k,l} Z_{k+1,l} + Z_{k,l} Z_{k,l+1})$$

With the same neglected terms as above, the condition sum becomes:

$$Z = e^{\frac{nN^2}{2}(nI + \mu H)} \left(\frac{\hbar\theta}{In} \right)^{N^2} \frac{\pi^{N^2}}{\prod_{k,l} A_{k,l}}$$

The secular problem for the determination of the $A_{k,l}$ is:

$$-\frac{1}{2}(u_{k-1,l,\mu} + u_{k,l-1,\mu}) + (2 + a - A_{k,l}) u_{k,l,\mu} - \frac{1}{2}(u_{k+1,l,\mu} + u_{k,l+1,\mu}) = 0.$$

The solutions are:

$$u_{k,l,\mu} = e^{\frac{2\pi i}{N}(kl + l\mu)} \\ A_{k,l} = 2 + a - \cos \frac{2\pi}{N} kl - \cos \frac{2\pi}{N} l\mu$$

We set:

$$\frac{2\pi}{N} kl = \xi ; \quad \frac{2\pi}{N} l\mu = \eta$$

and obtain for the logarithm of the condition sum:

$$\ln Z = \frac{N^2 n}{\theta} (nI + \mu H) + N^2 \ln \frac{\hbar\pi\theta}{nI} - \left(\frac{N}{2\pi} \right)^2 \int \int \ln (2 + a - \cos \xi - \cos \eta) d\xi d\eta$$

The expected value for the magnetic moment thus becomes for the layer lattice:

$$\bar{\mu} = N^2 n\mu - \left(\frac{N}{2\pi} \right)^2 \frac{\mu\theta}{nI} \int \int \frac{d\xi d\eta}{2 + a - \cos \xi - \cos \eta}$$

and in an analogous manner for the space lattice:

$$\bar{\mu} = N^3 n \mu - \left(\frac{N}{2\pi}\right)^3 \frac{\mu \theta}{n l} \iiint \frac{d\xi d\eta d\zeta}{3 + a - \cos \xi - \cos \eta - \cos \zeta}$$

For $\alpha \rightarrow 0$, only the space lattice retains a finite saturation:

$$\left. \begin{aligned} \bar{\mu}_s &= N^3 n \mu (1 - a \theta) ; \\ a &= \frac{1}{2 l n^3} \left(\frac{1}{2\pi}\right)^3 \iiint \frac{d\xi d\eta d\zeta}{\sin^2 \frac{\xi}{2} + \sin^2 \frac{\eta}{2} + \sin^2 \frac{\zeta}{2}} \end{aligned} \right\} \dots (12)$$

while the quantum-mechanical calculation resulted in

$$\mu_s = N^3 n \mu (1 - a' \theta'^2)$$

This calculation shows that the ferromagnetism is not a typical quantum-mechanical effect. While the magnetic saturation at low temperatures is considerably enhanced by quantum effects, it also occurs in the "classical" consideration, under the same conditions, as in the Bloch calculation.

As already noted by Bloch, (12) contradicts the Nernst law of thermodynamics. It is reasonable to provide relief through subsequent quantizing, in a process analogous to the Debye theory of specific heat.

3. The Quantizing of Spin Waves

With small deviations X_i and Y_i of the magnetic moments from the field direction, the coordinates $p_i = \sqrt{\frac{n\hbar}{2}} X_i$ and $q_i = \sqrt{\frac{n\hbar}{2}} Y_i$ are conjugated canonically. We obtain a new system of canonical variables in that we subject p_i and q_i to contragredient transformations. In accordance with (7), we select U real and form

$$p_i = \sum u_{ik} p'_k \quad q_i = \sum (U^{-1})_{ik} q'_k = \sum u_{ki} q'_k$$

In the eliminated variables, we obtain for the energy of the linear chain:

$$W = -Nn \left(\frac{nI}{2} + \mu H \right) + \frac{In}{h} \sum_{\lambda=1}^N \left(1 + a - \cos \frac{2\pi \lambda}{N} \right) (p_{\lambda}^2 + q_{\lambda}^2)$$

As this equation shows, our system is a harmonic oscillator in each of the N pairs of variables $p'_{\lambda}, q'_{\lambda}$, namely with the frequency:

$$\omega_{\lambda} = \frac{2In}{h} \left(1 + a - \cos \frac{2\pi \lambda}{N} \right) \dots \dots \dots (13)$$

Each magnetic condition of the lattice near the absolute saturation can be considered as superposition of "spin waves" of these fundamental frequencies.

An eigenvalue of the entire system is obtained by ascribing an arbitrary quantum number n_{λ} to each oscillator ω_{λ} :

$$E_{n_1, n_2, \dots, n_N} = -Nn \left(\frac{nI}{2} + \mu H \right) + \sum_{\lambda=1}^N n_{\lambda} \hbar \omega_{\lambda} \dots \dots (14)$$

Equation (14) contains all eigenvalues of the system. According to (2), we calculate the condition sum:

$$Z = \sum_{n_1=0}^{\infty} \dots \sum_{n_2=0}^{\infty} \dots \sum_{n_N=0}^{\infty} e^{-\frac{E_{n_1, \dots, n_N}}{\theta}}$$

According to (14), we have:

$$\begin{aligned} Z &= e^{+\frac{Nn \left(\frac{nI}{2} + \mu H \right)}{\theta}} \prod_{\lambda=1}^N \sum_{n_{\lambda}=0}^{\infty} e^{-\frac{n_{\lambda} \hbar \omega_{\lambda}}{\theta}} \\ &= e^{\frac{Nn \left(\frac{nI}{2} + \mu H \right)}{\theta}} \prod_{\lambda=1}^N \frac{1}{1 - e^{-\frac{\hbar \omega_{\lambda}}{\theta}}} \\ \ln Z &= \frac{Nn}{\theta} \left(\frac{nI}{2} + \mu H \right) - \sum_{\lambda=1}^N \ln \left(1 - e^{-\frac{\hbar \omega_{\lambda}}{\theta}} \right) \end{aligned}$$

We introduce the ω_λ according the (13) and again replace the sum by an integral:

$$\ln Z = \frac{Nn}{\theta} \left(\frac{nI}{2} + \mu H \right) - \frac{N}{2\pi} \int_0^{2\pi} \ln \left(1 - e^{-\frac{2In}{\theta} (1 + a - \cos \xi)} \right) d\xi$$

The expected value of the magnetic moment for the linear chain now becomes:

$$\bar{\mu} = Nn\mu - \left(\frac{N}{2\pi} \right) 2\mu \int_0^{2\pi} \frac{d\xi}{e^{\frac{2In}{\theta} (1 + a - \cos \xi)} - 1}$$

The analogous calculation results in:

$$\bar{\mu} = N^2 n\mu - \left(\frac{N}{2\pi} \right)^2 2\mu \int_0^{2\pi} \int_0^{2\pi} \frac{d\xi d\eta}{e^{\frac{2In}{\theta} (2 + a - \cos \xi - \cos \eta)} - 1}$$

for the layer lattice and

$$\bar{\mu} = N^3 n\mu - \left(\frac{N}{2\pi} \right)^3 2\mu \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \frac{d\xi d\eta d\zeta}{e^{\frac{2In}{\theta} (3 + a - \cos \xi - \cos \eta - \cos \zeta)} - 1}$$

for the space lattice.

This is exactly the formula of Møller if the integral is still evaluated by the series

$$\cos \xi = 1 - \frac{\xi^2}{2} \dots$$

In this connection, it is perhaps not uninteresting to note that the Møller calculation can be interpreted in such a way that only those condition of the lattice are taken into consideration in which almost all atoms in the direction of the magnetic field possess the spin moment $\frac{n}{2} \hbar$ and the few remaining ones the spin moment $\left(\frac{n}{2} - 1 \right) \hbar$, thus only less by one quantum number. In the classical picture, the assumption thus corresponds that the spin directions deviate only little from the field direction.

The complete agreement of the above calculation with the theory of Bloch results in a very clear interpretation of the Bloch spin waves. Their carrier is a system of spins elastically coupled by exchange forces. An excitation of the n -th quantum condition of the classically calculated eigenfrequency

$$\omega_{\lambda\mu} = \frac{2In}{\hbar} \left(3 + a - \cos \frac{2\pi}{N} x - \cos \frac{2\pi}{N} \lambda - \cos \frac{2\pi}{N} \mu \right).$$

corresponds to the condition that n spin deviations according to the De Broglie wave

$$e^{\frac{2\pi i}{N} (kx + l\lambda + m\mu)}$$

wander through the lattice.

The Bose statistic of the elastic natural oscillations is identical with the Bloch "sum of Bose gases".

However, it should be noted that the exact agreement of our calculation with the results of Bloch and Møller was hardly clear from the start because the normal coordinates p'_λ, q'_λ do not at all correspond to well-defined quantum-mechanical operators. This is probably due to the fact that we had to omit the null point energy in (14) in order to arrive at agreement with the quantum-mechanical calculation with regard to the absolute value of the energy and of the magnetic saturation.